High-Fidelity Multi-Phase Radiation Module for Modern Coal Combustion Systems

Michael F. Modest

Shaffer and George Professor of Engineering
University of California Merced
Merced, CA 95343, USA

DE-FG26-10FE0003801

June 8, 2011 — Pittsburgh

Radiation Challenges in Multi-Phase Reacting Flows

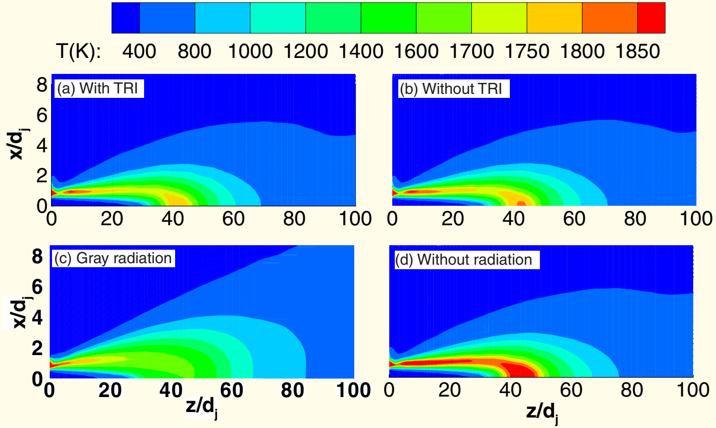
- Radiative heat transfer in high temperature combustion systems
  - Thermal radiation becomes very important at elevated temperatures
  - Coal and hydrocarbon fuels $C_nH_m \rightarrow H_2O$, CO_2, CO, NO_x, soot, char, ash
  - CO_2, H_2O, soot, char and ash strongly emit and absorb radiative energy (lower temperature levels)
  - Radiative effects are conveniently ignored or treated with very crude models
    - Neglecting radiation $\Rightarrow$ temperature *overpredicted* by several hundred °C
    - "optically-thin" or gray radiation $\Rightarrow$ temperature *underpredicted* by up to 100°C
    - Neglecting turbulence–radiation interactions $\Rightarrow$ temperature overpredicted by 100°C or more
    - In contrast: simple *vs.* full chemical kinetics $\Rightarrow$ same overall heat release and similar temperature profiles

Radiation Challenges in Multi-Phase Reacting Flows

- Radiative heat transfer in high temperature combustion systems
  - Thermal radiation becomes very important at elevated temperatures
  - Coal and hydrocarbon fuels $C_nH_m \longrightarrow H_2O$, CO_2, CO, NO_x, soot, char, ash
  - CO_2, H_2O, soot, char and ash strongly emit and absorb radiative energy (lower temperature levels)
  - Radiative effects are conveniently ignored or treated with very crude models
    - Neglecting radiation $\Rightarrow$ temperature *overpredicted* by several hundred °C
    - "optically-thin" or gray radiation $\Rightarrow$ temperature *underpredicted* by up to 100°C
    - Neglecting turbulence–radiation interactions $\Rightarrow$ temperature overpredicted by 100°C or more
    - In contrast: simple *vs.* full chemical kinetics $\Rightarrow$ same overall heat release and similar temperature profiles

Radiation Challenges in Turbulent Combustion

Computed temperature contours for Sandia Flame D scaled-up $4\times$



In presence of coal radiation expected to be stronger, but more gray; TRI unknown

State of the Art of Radiation Modeling

- Radiative Transfer Equation (RTE) Solvers
  - DOM/FVM included in CFD codes (ray effects, poor for optically thick media, high orders expensive)
  - SHM/*P–N*: *P–1* in CFD codes (cheap and powerful; poor for optically thin media); higher orders (*P–N*) complex
  - Photon Monte Carlo (very powerful; expensive, statistical scatter); ideal for stochastic turbulence models
  - *P–1* ideal solver for optically thicker pulverized coal/fluidized beds
- Spectral Models
  - Full-spectrum k-distributions (very efficient; cumbersome assembly, species overlap issues)
  - Line-by-line Monte Carlo module (outstanding accuracy at small additional cost)
- Turbulence–Radiation Interactions
  - Hybrid RANS-FV/transported PDF Monte Carlo
  - Emission TRI resolved with conventional RTE solver (OTFA)
  - Full TRI resolved with photon Monte Carlo for stochastic media

Research Objectives

1. Spectral radiation properties of particle clouds
    - coal, ash, lime stone, etc.,
    - varying size distributions and particle loading
    - classified, pre-evaluated and stored in appropriate databases
2. Spectral radiation models for particle clouds
    - Adapt high-fidelity spectral radiation models for combustion gases
    - Extensions to large absorbing/emitting–scattering particles in fluidized bed and pulverized coal combustors
    - New gas–particle mixing models and consideration of scattering
3. RTE solution module
    - *P–1* (and perhaps a *P–3*) solver (for optically thick applications)
    - Photon Monte Carlo solver (for validation and for optically thinner applications)
4. Validation of Radiation Models
    - Module connected to MFIX and OpenFOAM
    - Comparison with experimental data available in the literature
    - Simulations for fluidized beds and pulverized-coal flames

Research Objectives

1. Spectral radiation properties of particle clouds
   - coal, ash, lime stone, etc.,
   - varying size distributions and particle loading
   - classified, pre-evaluated and stored in appropriate databases
2. Spectral radiation models for particle clouds
   - Adapt high-fidelity spectral radiation models for combustion gases
   - Extensions to large absorbing/emitting–scattering particles in fluidized bed and pulverized coal combustors
   - New gas–particle mixing models and consideration of scattering
3. RTE solution module
   - *P–1* (and perhaps a *P–3*) solver (for optically thick applications)
   - Photon Monte Carlo solver (for validation and for optically thinner applications)
4. Validation of Radiation Models
   - Module connected to MFIX and OpenFOAM
   - Comparison with experimental data available in the literature
   - Simulations for fluidized beds and pulverized-coal flames

Research Objectives

1. Spectral radiation properties of particle clouds
   - coal, ash, lime stone, etc.,
   - varying size distributions and particle loading
   - classified, pre-evaluated and stored in appropriate databases
2. Spectral radiation models for particle clouds
   - Adapt high-fidelity spectral radiation models for combustion gases
   - Extensions to large absorbing/emitting–scattering particles in fluidized bed and pulverized coal combustors
   - New gas–particle mixing models and consideration of scattering
3. RTE solution module
   - *P–1* (and perhaps a *P–3*) solver (for optically thick applications)
   - Photon Monte Carlo solver (for validation and for optically thinner applications)
4. Validation of Radiation Models
   - Module connected to MFIX and OpenFOAM
   - Comparison with experimental data available in the literature
   - Simulations for fluidized beds and pulverized-coal flames

Research Objectives

1. Spectral radiation properties of particle clouds
   - coal, ash, lime stone, etc.,
   - varying size distributions and particle loading
   - classified, pre-evaluated and stored in appropriate databases
2. Spectral radiation models for particle clouds
   - Adapt high-fidelity spectral radiation models for combustion gases
   - Extensions to large absorbing/emitting–scattering particles in fluidized bed and pulverized coal combustors
   - New gas–particle mixing models and consideration of scattering
3. RTE solution module
   - *P–1* (and perhaps a *P–3*) solver (for optically thick applications)
   - Photon Monte Carlo solver (for validation and for optically thinner applications)
4. Validation of Radiation Models
   - Module connected to MFIX and OpenFOAM
   - Comparison with experimental data available in the literature
   - Simulations for fluidized beds and pulverized-coal flames

Spectral Radiation Properties of Particle Clouds

Particle spectral properties governed by complex index of refraction $(m = n - ik)$

1. Coal
   - Gray over short wavelengths $(1 \sim 6\mu\text{m})$, both n and k increase slightly for longer wavelengths $(6 \sim 10\mu\text{m})$
   - Value varies with type
2. Char
   - Both n and k increase weakly with wavelength
3. Ash
   - Fairly constant refractive index (n)
   - Absorptive index(k) depends on mineral constituents
4. Limestone
   - Has three absorption bands (Querry *et al* 1978)
5. Soot
   - Polynomial expression (Chang and Charalampopoulos 1990)

Spectral Radiation Properties of Particle Clouds, cont'd

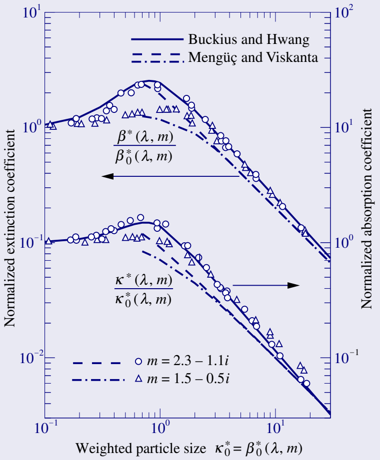
Absorption/extinction coefficients normalized by Rayleigh limit

- independent of particle size distributions
- dependent on a mean particle diameter
- may be applied to all solid phases in MFIX

Absorption and scattering coefficient database

- absorption coefficient: stepwise gray for each of the 248 narrow bands for combustion gases
- scattering coefficient: gray scattering
- allowance for user-defined values

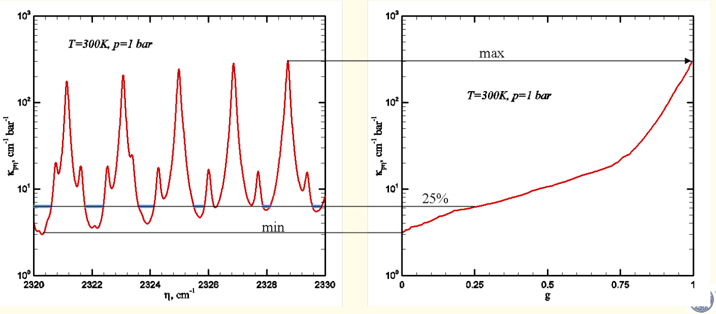
Coal Radiative Properties



Spectral Models for Combustion Gases

Narrow Band *k*-Distributions

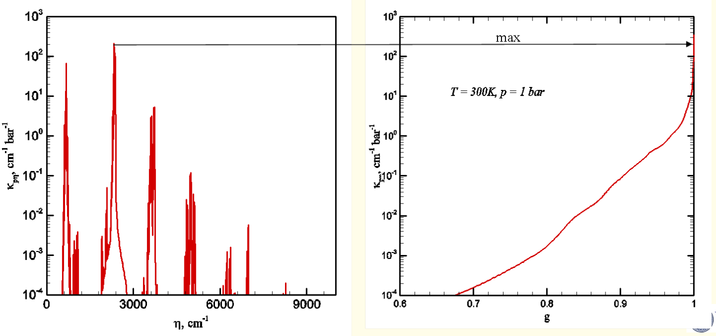
- RTE (without scattering): $\dfrac{dI_\eta}{ds} = \kappa_\eta \left(I_{b\eta} - I_\eta\right)$
- Planck function much better behaved than absorption coefficient, $\approx$ const over small part of spectrum $\Delta\eta$
- Can be reordered into a monotonically increasing function
- On right cumulative *k*-distribution of narrowband spectrum on left
- Requires "correlated" absorption coefficient



Spectral Models for Combustion Gases, cont'd

Full-Spectrum k-Distribution

- On right cumulative full-spectrum k-distribution of CO_2 absorption coefficient at 300 K, 1 bar on left
  - Very steep at k_{max}
  - Covers many orders of magnitude
  - Part of spectrum has "zero" κ_η
  - 6–10 RTE evaluations as opposed to $>$1,000,000 for LBL
  - Requires "correlated" absorption coefficient



Capabilities of MFIX and OpenFOAM

	MFIX	OpenFOAM
Gas-particle multiphase flow		
Dense	Full Support	None
Dispersed	Full Support	Lagrangian
Model Approach		
Continuum	Full Support	General
Discrete	DEM	Lagrangian Particle
Grid	Cartesian, Cylindrical	Unstructured
Physics		
Turbulence	$k - \epsilon$	Full Support
Radiation	T^4 law	Gray P-1

RTE Solution Module

P–1 Solver:

- Ideal RTE solver for expected large optical thicknesses
- Single-scale full-spectrum k-distribution, assembled from narrow-band data for particulates and gas k-distributions
- One RTE solution, but separate emission and absorption terms for individual phases

Photon Monte Carlo Solver

- Ported from our gas combustion work with LBL module
- Particulate emission and absorption added
- To ascertain accuracy of *P–1*/replace it whenever necessary

Validation of Radiation Module

- Standard validation against "exact" solutions for simple problems
- Comparison of MFIX vs. OpenFOAM for problems solvable by either (pulverized coal combustion)
- Comparison with experiment
  - added simulation tools to directly compute measured data
- Case studies

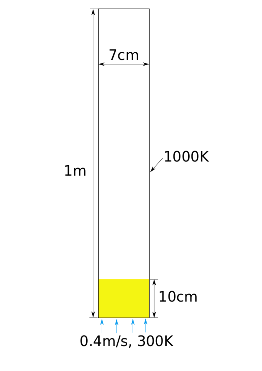
Work to Date

- MFIX installation
  - Installed on Cluster (64bit) and PC (32bit)
  - Set up test runs of fluidized bed and dilute gas-particle flows
  - Set up test runs of $k - \epsilon$ turbulence model
- *P–1* module
  - Rewrite discretization subroutines for PDE and boundary conditions
  - Gray participating media
  - Gray boundary conditions
  - Spatial varying absorption coefficients
- Radiative property database
  - Surveyed experimental measurements of radiative properties of particles in coal combustion
  - Compiled radiative properties of particles in coal combustion
  - Started to port gas property database to MFIX

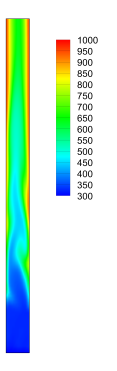
Work to Date, cont'd

Test for *P–1* module in a fluidized bed

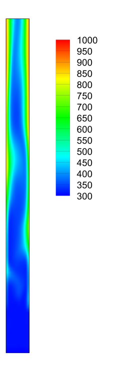
- Black wall $T_w = 1000\text{K}$
- Gray gas and particle $\beta_g = \kappa_g = 0.1\text{m}^{-1}$, $\beta_s = \kappa_s = 20\text{m}^{-1}$
- Single particle size $d_s = 0.4\text{mm}$



Gas phase temperature at $t = 40\text{s}$



With Radiation

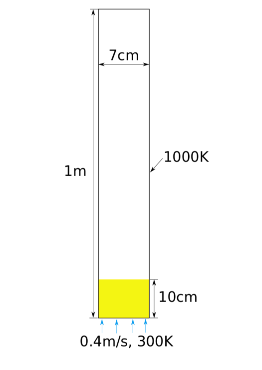


Without Radiation

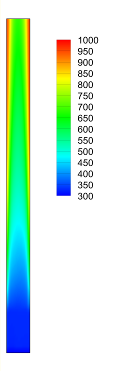
Work to Date, cont'd

Test for *P–1* module in a fluidized bed

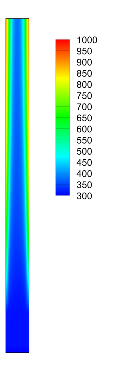
- Black wall $T_w = 1000\text{K}$
- Gray gas and particle $\beta_g = \kappa_g = 0.1\text{m}^{-1}$, $\beta_s = \kappa_s = 20\text{m}^{-1}$
- Single particle size $d_s = 0.4\text{mm}$



Gas phase temperature time averaged



With Radiation



Without Radiation

Effort for Next Year

- Spectral Models for Solid Particles
  - k-distributions for particles
  - mixing models
- RTE Solvers for Solid Particle–Gas Mixtures
  - Completion of *P–1* module
  - Implementation of PMC solver
  - spectral module for PMC solver
- Validation of Radiation Module
  - Literature survey of experimental data
  - Setup of simulations against experimental data
  - Parametric runs of relevant combustors